BRIJUNI INTERNATIONAL CONFERENCES ON INTERDISCIPLINARY TOPICS IN SCIENCE VI.

END OF CENTURY STATE OF SCIENCE

September 7-12, 1998
BRIJUNI, CROATIA

We wish to thank the following for their contribution to the success of this conference

Ruđer Bošković Institute, Zagreb
Ministry of Science and Technology, Croatia
United States Air Force European Office of Aerospace Research and Development
Royal Society, London
National Park Brijuni, Brijuni
Wolfram Research Inc., USA
Systemcom. d.o.o., Zagreb

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	12 September 1998	Conference Proceedings

4. TITLE AND SUBTITLE

END OF CENTURY STATE OF SCIENCE

5. FUNDING NUMBERS

F6170898W0008

6. AUTHOR(S)

Conference Committee

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

R. Boskovic Institute
Bijenicka c. 54
Zagreb 10001
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8. PERFORMING ORGANIZATION REPORT NUMBER

N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

EOARD
PSC 802 BOX 14
FPO 09499-0200

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

CSP 98-1008

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

A

13. ABSTRACT (Maximum 200 words)

The Final Proceedings for END OF CENTURY STATE OF SCIENCE, 7 September 1998 - 11 September 1998

This is an interdisciplinary conference. Topics include Ultracold collisions, Early Universe Computer power, Complexity of biological systems, the ultimate constituents of matter, Molecules in Space, Atoms, molecules, clusters, solids and Radiation-matter interaction

14. SUBJECT TERMS

EOARD, Physics, Chemistry, Biology

15. NUMBER OF PAGES

45

16. PRICE CODE

N/A

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

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2. Abstracts

Exact quantum mechanics near the classical hyperquantization algorithm for reactivity and structure

Vincenzo Aquilanti

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Harmonic analysis generalizes Fourier expansions and transforms, and we develop it in order to provide efficient computational implementation to the particularly demanding cases of atomic and molecular physics where the density of states is high. Physically, wavefunctions for the angular part of the kinetic energy operator are spherical harmonics, i.e. eigensolutions to Laplace operator on the ordinary sphere: they add and multiply according to the rotation group operations, so providing the framework for the quantum theory of angular momentum (Clebsch-Gordan Series, sum rules for 3-j and 6-j coefficients...).

The mathematical tools are the classical orthogonal polynomials as well as their discrete analogues (hyperquantization algorithm). The computational advantages are due to the existence of closed form expressions, three-term recurrences, analytical integrals. Work is presented here on multidimensional extensions, to treat exactly chemical reactions including spin and electronic angular momenta [(J. Chem. Phys., **108**, in press, 1998) and references therein].

For many-body problems, the kinetic energy operators, when conveniently written in hyperspherical coordinates, have as eigensolutions hyperspherical harmonics, which can be interpreted as wavefunctions of hyperangular momenta, whose algebra, which is within the boundaries of Gauss' hypergeometric function theory, is being developed.

Hyperharmonics can also be exploited as atomic and molecular orbitals, extending Fock projection into momentum space for the hydrogen atom to the n-dimensional case, and introducing alternative expansions for a multidimensional plane wave, of use for generalized Fourier transforms. This method allows us to work both in configuration space (on eigenfunctions expanded on a Sturmian basis) and in momentum space (on a (n + 1) dimensional hyperspherical harmonics expansions) [(Phys. Rev. Lett., **80**, 3209, 1998) and references therein].

LiH the molecule with many applications

Ticijana Ban, Hrvoje Skenderović and Goran Pichler

Institute of Physics, 10000 Zagreb

Croatia

LiH molecule is the simplest metal hydride with extremely large permanent dipole moment. Its energy structure and spectroscopy is not well known, and only quite recently several theoretical and experimental investigations shed a new light on this probably one of the oldest (primordial) molecule. We shall describe results of spectral behaviour of LiH molecules in neutral vapor and low pressure electric discharge in specially designed heat-pipe ovens, with emphasize to several applications.

Molecules in Intense Laser Fields:

Enhanced Ionization, Harmonic Generation, and Coulomb Explosions; Exact Simulations

A.D. Bandrauk and B. Schelkowski

Laboratoire de Chimie Theorique,

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Numerical solutions of the time-dependent Schroedinger equation have been obtained for one and two-electron quantum proton "wires": $H_{n,n}$=2-5.These exact simulations demonstrate the existence of a new molecular-strong field phenomenon not encountered in single atoms under similar conditions: Charge Resonance Enhanced Ionization-CREI, and enhanced high order Harmonic Generation into the VUV-X-Ray region. Interpretation of these unusual nonlinear non-perturbative optical phenomena will be shown to be possible using simple classical plasma physics concepts. Finally an exact non-Born-Oppenheimer calculation has been realized for the H_2^+ system allowing for the calculation of Above Threshold Ionization, ATI, electron and nuclear Coulomb explosion spectra simultaneously. These new results will be shown to lead to a new molecular imaging technique: Laser Induced Coulomb Explosion Imagery-LICEI. Possible early experimental results form PBCorkum's NRC (Ottawa) laboratory will be shown.

Optical magnetic double resonance control of atom-molecule composition of metal vapors

R. A. Bernheim

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Optical pumping of Na atoms with polarized laser radiation tuned to one of the atomic resonance transitions produces a shift in the vapor phase atom-dimer equilibrium densities. The direction of the shift is determined by the polarization of the light. Besides the already known decrease in equilibrium Na_2 vapor density resulting from Na atomic orientation produced by circularity polarized D_1 light, an increase in Na_2 density is produced when the excitation is changed to plane polarized radiation at either the D_1 or D_2 transition energy. While there are several possible mechanisms for this latter effect, the evidence seems to point toward a reaction between Na ($2P_{1/2}$ or $2P_{3/2}$) atoms and Na ($2S_{1/2}$) ground state atoms to form dimers in several electronically excited states which then either radiate or follow dark processes to produce additional ground state dimer density. It is now possible to change the gas phase atom-dimer bulk equilibrium composition to favor either products or reactions by a simply changing the laser polarization and power used for the atomic excitation. When optically pumping with circularly polarized D_1 radiation, it is also demonstrated that saturation of the ground state Na atomic Zeeman magnetic resonance transition not only reverses the decrease in equilibrium density of Na_2, but also produces an increase above the normal thermal value. The magnetic resonance transition can, therefore, be used to control both the direction and extent of the shift in equilibrium composition.

Topographies and Dynamics in Many Dimensions: Clusters and Protein Models

R. Stephen Berry

Department of Chemistry and the James Franck Institute

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Chicago, IL 60637, USA

Efficient computational tools allow us to catalogue the stationary points and topographies of systems of as many as 12-15 particles, but to interpret larger systems, we must use statistical methods. Databases whose elements are sequences of adjacent minima, connected by the saddle points between them, provide the information to carry out such interpretations. Generalizations that emerge are these: sawtooth-like topographies appear to be associated with short-range potentials, with few-particle motions from one minimum to the next and with easy formation of amorphous structures, while staircase-like potentials arise from long-range interactions, highly collective well-to-well motions and strong structure-seeking character, whether crystallizing or folding. The information about the sequences of stationary points allows us to construct master equation for the time evolution of arbitrary distributions on the surface and to determine optimal temperature programs to approach target distributions of particle energies and morphologies.

The tale of QT

S. Danko Bosanac

Ruđer Bošković Institute, 10000 Zagreb, Croatia

A brief account of the development of quantum theory is made. Its roots can be almost entirely connected with the study of interaction of electromagnetic field with matter. From the start the assumption was that connection with classical theory should be severed, and new theory must be based on entirely new basis. In the recent studies quantum theory is formulated from classical, by adding a new postulate to the three Newton´s. On the example of angular momentum for a free particle it is shown how this approach gives entirely new view about its nature.

Modelling the formation of a protogalaxy

S. Danko Bosanac[1], W. Klemperer[2] and F. Scappini[3]

[1]Ruđer Bošković Institute, Zagreb, Croatia

[2]Harvard University, Cambridge, MA 02138, USA

[3]Istituto di Spettroscopia Molecolare, CNR, Bologna 40129, Italy

Formation, dynamics and thermal evolution of a collapsing proto-cloud, which was formed after the recombination epoch, is investigated. The mass of the proto-cloud is divided into fragments and their time evolution is followed. The initial conditions for the fragments are taken randomly in order to simulate fluctuations in the density of the cloud. It is shown that after the initial, fast, collapse about one third of the mass is ejected, the remaining core being cooled to a relatively low temperature. After ejection of matter the core has angular momentum, and the hypothesis is that it prevents additional fast collapse of the cloud.

Exploring complexity from simplicity: Clusters

Udo Buck

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Small clusters are usually thought to behave like molecules, while the larger ones are considered to show properties of the condensed solid or liquid. A critical indication of such a behavior is the transition from single to collective excitations in the clusters. We will present recent experimental examples and discuss possible changes caused by the finite number of particles. The examples will include with decreasing excitation energies: plasmons for metal clusters, intramolecular vibrations for hydrogen bonded networks, translational motions (phonons) for weakly bound systems, and, finally, rotons for superfluid helium clusters.

The role of technology in the evolution of science

Wilfrid Claeys

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In 1610, the telescope allowed Galilee to discover the main satellites of Jupiter. In 1995 the Galileo space probe allowed the study of the internal structure of these satellites. These two situations, separated by nearly four centuries, are two examples of the important role of technology in unexpected discoveries. Technology and instrumentation are part of the scientific process on the same level as theory and experimentation.

I will take advantage of my own experience in optoelectronics to illustrate how technological developments can open new areas for fundamental research. My research group develops optical characterization methods for integrated circuits. With an instrumental concept from the 19^{th} century coupled with nowdays laser technology and detection electronics, we have been able to measure surface displacements in the 10^{-15} m (femtometer) range. This very powerful instrumentation allowed us to see the "breathing" of running electronic components. This "breathing" process, not yet fully explained theoretically, opens new fields for fundamental research.

Many other similar and more important developments could serve to illustrate the extraordinary possibilities opened by technological developments. Amongst the major ones let us just quote the following: the transistor and associated electronics and computers, lasers, atomic force and near field microscopes, ...

By the end of this century we observe that more and more money is put in applied research; private companies develop instrumentation and our major funding organizations tend to direct us towards applied work. This trend is worth a discussion.

The role of chemical reaction dynamics calculations

David C. Clary

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Experiments on chemical reaction dynamics aim to study the details of reactions beyond just simple rate constants at room temperature. Reactant and product molecules can have different translational energies, varying angles of orientation and different internal quantum states. Developing experiments to study such microscopic aspects of chemical reactions has become a major area of physical chemistry. Why is it worthwhile doing calculations on chemical reaction dynamics? This talk will answer this question. It will be shown that: 1. Calculations have matured so that they can predict the results of new experiments with confidence. 2. Calculations can help interpret experiments when the results are puzzling. 3. Reaction dynamics calculations can have useful applications for modelling conditions that are hard to produce in the laboratory. Understanding problems in atmospheric, combustion and interstellar chemistry are good examples of this. These three points will be illustrated with recent examples from our group of reaction dynamics calculations done using quantum scattering methods [1].

1. D. C. Clary, Science **279**, 1879 (1998).

Molecules in the Early Universe

Alex Dalgarno

ITAMP at Center for Astrophysics and Harvard University

60 Garden Str., Cambridge, MA 02138, USA

A discussion will be given of the mechanisms involved in the formation and destruction of molecules and their possible detection in the early universe and in the first cosmological objects. There have been several calculations of the molecular abundance as functions of the red shift with some differences. New results will be presented and the differences resolved.

Issues in particle physics and the LHC project

Daniel Denegri

CERN

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Switzerland

We discuss some of the major issues in particle physics to be addressed in the coming years, in particular with the advent of the Large Hadron Collider (LHC) project at CERN. We present the present status of the machine, of the major experiments, more specifically of the general purpose CMS (Compact Muon Solenoid) experiment, with the prospects for Higgs boson searches, for electroweak scale Supersymmetry and CP violation studies in the B sector.

Control Schemes for Laser Driven H-atom Switching in the Condensed Phase

Nađa Došlić*

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Berlin D-14195, Germany

During the last decade different schemes for controlling chemical reactions by means of tailored laser pulses have been developed. While most of the theoretical and experimental work done so far deals with isolated molecules in the gas phase it is challenging to investigate these ultra fast dynamical processes under condensed phase conditions. There the laser control is counteracted by energy dissipation processes which tend to move the system into thermal equilibrium.

In the present work we study the ultra fast photoisomerization dynamics of intramolecular hydrogen transfer systems. We will show how different schemes for controlled hydrogen switching perform in the presence of dissipation. The hydrogen transfer is modelled in terms of a low dimensional system weakly coupled to a Markovian heat bath. For the energy surface along the reaction co-ordinates we use model potentials with parameters adjusted to (ab initio) data obtained for different molecules (e.g. malonaldehyde derivatives). The dynamics on these potential surfaces is simulated using density matrix theory. Among the control schemes we investigate are the pump-dump approach and different variants of the recently proposed "hydrogen subway" scheme for tunnelling control.

A formal model of evolution in connection with protein folding theory

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A common feature of the traditional approaches of both title theories is the assumed presence of many secondary maxima in Sewall-Wright's landscape and of many secondary minima in the potential hypersurfaces of proteins. The former assumption results in assigning a major role to environmental changes (including possible coevolution, as well as isolation) in the evolution from a species to a new one; the latter favors kinetic and thermodynamic behaviors of protein folding which actually are not observed.

In contrast, we find strong evidence for a negligible presence of secondary maxima or minima in hypersurfaces of homogeneous nature and with a high number of degrees of freedom: most intermediate 'states' should be saddle points of various orders, out of which the systems escapes along a normal mode with low, imaginary frequency. If this is true, protein folding essentially is a random - walk, slightly 'downward'-biased, negentropy-controlled process, whereas evolution proceeds from a given species along neutral, low probability lines in mutation space. Hints on the connectivity between such evolutionarily neutral islands may be borrowed from the study of 'designability' of protein folds, either in reality or on simple computer models of proteins.

Exobiology: origin, evolution and distribution of life in the Universe

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General definition of exobiology is the study of life in the Universe. More precisely it includes:

- the study of conditions and processes which have lead to the emergence of life in our planet. or which could have lead to it somewhere else
- the study of the evolution of organic matter from soimple to more complex structures in the Universe
- the research on the distribution of life under any form it could appear, and its evolution in the Universe

Recent developments in astronomy (discovery of extra solar planets, space exploration...) are at the origin of this new interdisciplinary field of research and we will present what could be the trails to follow to try to understand the origin of life.

Nanostructures:

A Discussion of Physical Properties and Phenomena, with Fullerenes as Examples

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Materials with dimensions on the nanometer scale, i.e., nanostructures, bridge the gap between molecules and solids. A wide variety of both experimental and theoretical studies have been carried out which look at various properties, e.g., structural and electronic, and associated physical phenomena. As an illustration, the specific examples of charge transfer and photoexcitation in fullerenes are discussed.

A generalized ring spiral algorithm for coding fullerenes and other cubic polyhedra

P. W. Fowler[a], A. Graovac[b], T. Pisanski[c] and J. Žerovnik[c,d]

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[c] University of Ljubljana, Ljubljana, Slovenia, [d] University of Maribor, Maribor, Slovenia

The so-called ring spiral algorithm is a convenient mean for generating and representing certain fullerenes and some other cubic polyhedra. In 1993 Manolopoulos and Fowler presented a fullerene on 380 vertices without a spiral. So smaller unspirable fullerene is known. In the spring of 1997 by using computer Gunnar Brinkmann found the smallest cubic polyhedron without a spiral. It has only 18 vertices. Here we generalize the ring spiral approach in order to obtain a canonical representation for arbitrary planar cubic polyhedra. Some other questions are addressed here like possible generalizations of this method to polyhedra of higher genus and to polyhedra with vertices of arbitrary valence.

Precision Spectroscopy of Atomic Hydrogen

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Recent advances in high-resolution laser spectroscopy and optical frequency metrology are making it possible to measure and compare optical transition frequency in atomic hydrogen with unprecedented precision. Recent experiments with hydrogen and deuterium are providing accurate new values for the Rydberg constant, the 1S ground state Lamb shift. and for the structure radius of the deuteron. Future work may unveil conceivable slow changes of fundamental constants or even differences between matter and antimatter.

The state of synergetics at the turn of the century

H. Haken

Theoretische Physik

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Modelling Interstellar Chemistry:

Why do Carbon Compounds Dominate the Observed Gas Phase Species?

Flavio Scappini and William Klemperer

Department of Chemistry

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We discuss molecule formation with a view towards treating the question of excess oxygen. We will discuss the stability of gas phase and solid phase species in the radiation fields that exist. We will also discuss molecular emission and high-energy molecular processes, in stellar envelopes.

Study of KZn excimer molecule

Irena Labazan , Svemir Rudić, Slobodan Milošević

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Study of simple diatomic intermetallic excimers as building blocks of nano structures could be important for technologies of the next century. Most of the alkali – IIB group excimer molecules have been observed and are well known, such as LiZn, LiCd, NaCd, KCd etc. [1]. The KZn excimer molecule has been predicted in theoretical ab initio calculations [2], but no experimental data were available so far. This is mainly due to the difficulties of preparing suitable vapour mixture. Here we use heat-pipe oven to prepare KZn amalgams with different mole ratio of potassium and zink. With classical absorption technique and fluorescence measurements we try to determine the best mole ratio for production of KZn.
It is very important to have small amount of potassium dimers in the vapour mixture because of spectral overlap of KZn C-X band with K_2 B-X band.
We study photoassociation (1) and photochemical (2) production of KZn excimer:

$$K + Zn + h\nu \text{ - } KZn^*$$

$$K_2^* + Zn \text{ - } KZn^* + K$$

Very low absorption coefficient of KZn molecule is detected with use of cavity ring down spectroscopy.

1. S. Milošević, Spectral Line Shapes, AIP Conf. Proc. No.328 (AIP New York, 1995). pp.391-405
2. E. Czuchaj, F. Rebentrost, H. Stoll, H. Preuss, *Chem. Phys. Lett.* **218,** 454-461 (1994)

Analysis and Control of Molecular Motion on a Femtosecond Timescale

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and R. Steven Berry*

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With the availability of ultrashort laser pulses, the analysis and control of chemical reactions on the femtosecond timescale has become possible. Our contribution will focus on various approaches to follow and ultimately drive a chemical reaction into a desired direction by the interaction of the molecular wave packet with tailor made light pulses. We will present recent examples from our laboratory.

The Attractors of Future

What do we want the XXI-st Century to be, and how?

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The attractors of nonlinear dynamics are well-known in the natural sciences. Complex systems in physics, chemistry, and biology seem to be driven by selforganizing forces near and far from thermal equilibria. Computer scientists are trying to simulate possible scenarios of virtual evolution and artificial life. Materials science, information networks, and biocomputing are highlights of complexity research at the turn of the century. It is now recognized that many of our social, economic, and political problems are also of a global, complex, and nonlinear nature. Are there concrete models of economical and social systems referring to the attractors of our civilization? How can they help solving complex problems of management, forecasting, and decision? But mastering the future does not only need an effective management. Ethical standards are demanded in a world with increasing complexity and dynamics.

The Physics of Elementary Chemical Processes: Newton or Schrödinger (or is Chemistry Simpler than we Thought)

Anthony McCaffery

University of Sussex, Brighton, UK

Recent experimental and theoretical studies of atom-diatom collision indicate that even the most highly resolved observations obey a hybrid Newtonian-Schrödinger mechanics in which the molecular eigenstates provide constraints to classical or near classical trajectories. Vector relations through which momentum of relative motion is converted to internal momentum of the molecule or into recoil are obeyed and thus the incident trajectory is set by the threshold requirements of the product $|v,j| >$ state.

This allows the development of easily visualised physical models from which quantitative predictions of the outcome of collions may be predicted. Models are described for inelastic and reactive collisions which successfully predict $|v,j| >$ distributions in the case of inelastic and reactive collisions. These vector conditions may be seen as an important component of the forces that determine stereochemistry in reactive encounters and incorporating such restrictions into the steric factor may lead to a re-evaluation of simple collision models of reaction rates.

Correlation:

How to make complicated things from simple ones

Jim McGuire

Tulane University,
New Orelans, LA, USA

One of the emerging question of science is how are complex things made from simple things? Larger is not necessarily more complicated than their smaller subsystems. In biology, chemistry and materials science the issue is how to understand large molecules in terms of atoms. In atomic physics one may strive to understand properties of many electron systems in terms of single electron properties. The general theme is interdependency of subsystems, or "correlation". Electron correlation dynamics is a central theme of this talk. The dynamics of electron correlation may affect single electron transitions. However, this effect is sometimes difficult to separate from other effects. Correlation is usually dominant in multiple electron transitions for fast collisions since there is not enough time for the collision partners to interact more than once. This means that multiple electron transitions in fast collisions provide an unobstructed view of the dynamics of electron correlation. Examples include double ionization of helium and other multiple electron transitions in interactions of atoms, molecules and earthworms in collisions with light and matter.

Nanolithography with laser cooled atoms

E. Jurdik and W.L. Meerts

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The Netherlands

Laser focusing of neutral atoms into a periodic array of nanometre-scale features has emerged as a promising method of nanostructure fabrication. Laser cooled atoms interacting with a near-resonant laser standing-wave created above the substrate are focused into nodes or antinodes of the light intensity depending on the sign of the detuning of the laser frequency from the atomic resonance, thus forming periodic nanostructures. The physics beyond this deposition technique involves processes governing the interaction of light with atoms as well as the surface diffusion phenomena. We study the nanostructure growth using a laser standing-wave as a mask within a semiclassical trajectory tracing approach. The effect of surface diffusion is incorporated due to a real-time stochastic model. The results are compared with experimental data for chromium deposition.

H_3^+ in Cosmic Plasmas

Takeshi Oka

Department of Astronomy and Astrophysics, and Department of Chemistry

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Because of the efficient ion-neutral reaction $H_2^+ + H_2 - H_3^+ + H$, the H_3^+ molecular ion is the most abundantly produced ion in H_2 dominated plasmas. The pure and intense H_3^+ emission spectrum from Jovian ionosphere has now been established as a useful probe for the study of its plasma activity [1]. Recently, H_3^+ with column densities of (1.7 - 5.5) x 10^{14} cm^{-2} has been detected in absorption towards the direction of young stellar objects GL2136, W33A, MonR IRS2, GL961E and GL2591 that are deeply embedded in molecular clouds [2,3]. Quite unexpectedly, H_3^+ with similar column density has also been detected in diffuse clouds toward the visible star Cygnus OB2 No. 12 [4], and with higher column density towards the Galactic Center [5]. The H_3^+ chemistry in these clouds with its astrophysical implication together with laboratory experiment on the conversion of ortho- and para- H_3^+ [6] will be discussed.

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A novel general formula for the hyper-Wiener index of acyclic structures

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The hyper-Wiener index was recently introduced by Randić. It is shown analytically that the hyper-Wiener index. the Wiener number and the W′/W index are closely related graph-theoretical invariants for acyclic structures. On the basis of this relationship the general analytical expression for the hyper-Wiener index of acyclic structures is derived. The formula provides an easy method to calculate the hyper-Wiener index for any connected acyclic graph.

Fundamental symmetries and the role of their violations in physics, chemistry, and biology:

The past 20th century and outlook to the next century

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Fundamental symmetries and their violations play a particular role in our understanding of nature. In the lecture we will start by out-lining some of the concepts in relation to molecular physics [1,2,3] in a very down to earth way, and then consider the consequences for and relationships to biology, physics and cosmology in a somewhat less down to earth perspective.

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Many Body Problems in Nuclear and Hadron Physics

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A remarkable achievement in theoretical physics has been the development of powerful many body techniques capable of quantitative description of important phenomena. I shall not speak here about the technical aspects of these calculations, nor about the elegant field-theoretical techniques (Feynman graphs): I shall rather concentrate on qualitative interpretation of several interesting situations.

1. Choice of relevant degrees of freedom. A beautiful example is the coexistence of collective and single-particle degrees of freedom. In nuclear physics these are the rotation (vibration) and single-nucleon motion. In hadron physics we have chiral dynamics (mesonic field) interacting with quarks (analogously as phonons interacting with polarons).

2. Fine tuning of natural constants. If masses of elementary particles and interactions between them were slightly different, life would not be possible. Many body effects often enhance such features. I shall present many picturesque examples.

3. Comparison of the shell structure in atoms, nuclei hadrons. Are three "generations" of quarks and leptons also some kind of shell structure.

Exploring Complexity from Simplicity:

Principles and Applications of Self-organizing Matter at the Nanoscale Level

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In this talk I hope to analyze the energetic, structural and kinetic foundations that stand at the basis of self-organization in many organic materials that self-assemble into ordered and useful structures at the nanoscale level. Some of these materials are useful model systems in the study of the behavior of matter in more complex (mostly biological) structures. Some others are being increasingly used for practical applications that range from the preservation and useful modification of technological surfaces and drug delivery to electronic and optoelectronic devices. Finally, some of these structures are simply beautiful constructs which we now fabricate and image with unprecedented detail in order to master these microscopic control techniques which are so young but, at the same time, so full of promise.

The average charge electrodynamics with heavy photons as a new neutral current interaction

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An approach of the unification of interactions in the n-dimensional coupling constant space associated with the gauge group SU(3) X SU(2) X G, where G is the generalization of U(1), is carried out. The result of this investigation is that the unification can proceed through two independent branches each having its own G. The requirement that they be physically equivalent can be easily achieved when the G for both branches is G = U(1)2 X .... X U(1)n, where the indices (1 to n) are associated with gauge coupling constants g1, g2, ... gn (g1 is the SU(2) gauge coupling constant). With the assumption that fermions have no other U(1) quantum numbers beyond the hypercharge quantum numbers, using the neutral current projections, unique to this approach, we conclude that the new neutral current interaction can be interpreted as the average charge electrodynamics with massive "photons". This result appears to be consistent with the recent precise measurement of parity violation on Cesium atom [1] as well as, already at a tree level, with the neutrino(s)-electron scattering. Presently, similar comparisons are carried out for other processes involving quarks.

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Making Molecules at MicroKelvin*

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The cooling and trapping of atoms and atomic ions is a rapidly advancing field of fundamental science (e.g. Bose-Einstein condensation). We are attempting to extend the field to neutral molecules (and also molecular ions) as well, e.g. for study of elastic, inelastic and reactive collisions in the highly quantum mechanical regime at extremely low energies. As a first step, we are employing single- and multicolor photoassociation to produce translationally ultracold $^{39}K_2$ molecules from ultracold (~300 μK) ^{39}K atoms confined in a magneto-optical trap.[1-7] Photoassociation of ultracold atoms (as opposed to thermal atoms) includes sharp resonances with wavelength as long-range rovibrational levels (outer turning points of tens or hundreds of Bohr) are accessed from colliding atomic pairs with <10 MHz of relative kinetic energy and only a few partial waves (l = 0, 1, 2). Potential energy curves derived from these spectra test electronic structure and long-range perturbation theory calculations of interatomic potentials. The molecules formed are translationally ultracold and rotationally cold.

Recently we have used two-color resonance enhanced multiphoton ionization to directly detect translationally ultracold molecules.[8] These molecules are formed in v'' = 36 of the ground $X^1\Sigma_g^+$ state of $^{39}K_2$ following spontaneous emission from v' ~ 191 of the $A^1\Sigma_u^+$ state, formed in turn by one-color photoassociation of ultracold ^{39}K atoms. In the near future, we will seek to produce translationally ultracold molecules in low rovibrational levels (v = 0-9, J < 3) of the $X^1\Sigma_g^+$ state via two-color photoassociation as proposed by Band and Julienne.[9] We plan as a further step to cool the rovibrational distribution of ground state translationally ultracold molecules produced by two-color photoassociation using laser cooling.[10]

We also plan to directly study free -- bound -- bound stimulated Raman photoassociation to directly produce state-selected translationally ultracold K_2 molecules as recently proposed.[11] Note the application of this technique to an atomic Bose-Einstein Condensate may yield a coherent beam of state-selected molecules[12] (a "molecule laser").

Finally we note that translationally ultracold molecules can also be produced in metastable electronic states (e.g. the $a^3\Sigma_u^+$ and $b^3\Pi_u$ states of the alkali dimers). Indeed Fioretti et al. have recently observed translationally ultracold Cs_2 $a^3\Sigma_u^+$ molecules using one-color resonance enhanced multiphoton ionization.[13]

* In collaboration with Professors Phil Gould and Ed Eyler, Drs. He Wang, John Bahns, Paul Julienne, Eite Tiesinga and Carl Williams, and Jing Li, Xiaotian Wang and Anguel Nikolov. Supported in part by the National Science Foundation.

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The Standard Model

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It will be sketched what the Standard Model {SM} contains and what it can describe. While the accent will be on the present status of SM, some general ideas which guide the construction of models beyond SM will be also mentioned.

Cold and Ultracold Collisions:

How Photons can Sew Atoms into Molecules and Nanostructures

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This talk will review theoretical and experimental developments in cold and ultracold collisions since there inception about ten years ago to their present role in quantum- statistical condensates. Optical control of inelastic processes and molecule formation will also be reviewed and future potential assessed.

ON THE DETOUR MATRIX

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A novel matrix in chemistry is detour matrix, known in the formal graph theory since 1969 (F. Harary, *Graph Theory* , Addison-Wesley, Reading, MA, 1969, p. 203). This matrix has been introduced in the chemical literature independently by two groups (O. Ivanciuc, A.T. Balaban, *Comm. Math. Chem.* **30** (1994) 141-152; D. Amić, N. Trinajstić, *Croat. Chem. Acta* **68** (1995) 53-62).

We will give the definition of the detour matrix and compared with the definition of the distance matrix. The computation of the detour matrix will be briefly outlined. Examples of graphs with identical detour matrices will be shown. We will consider three invariants of the detour matrix: the detour polynomial, the detour spectrum and the detour index. The detour matrix and its invariants will be derived for special classes of graphs such as cycles and complete graphs.

Diffuse bands and triplet satellite bands of Cs_2 molecule

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Many potential curves of cesium dimer molecule are heavily influenced by large spin-orbit splitting in the 6p atomic level. Among other effects it causes an interesting splitting structure in the first and the second excited $1\ ^3\Pi_g$ and $2\ ^3\Pi_g$ states. As a results of this we have instead of a single pair of $^3\Pi_g$ interacting potential curves (or avoided crossing) a more complex structure with 2_g, 1_g, 0_g^+ and 0_g^- pairs. The intensity borrowing and specific avoided crossing make the radiative transitions to the repulsive lower 1_u and 0_u^- states (they degenerate into a single $^3\Sigma_u^+$ lowest triplet potential curve).

In this contribution we shall discuss the origin of intensity structure of three diffuse bands and many satellite bands around 852.1 nm Cs resonance line. Calculated potential curves for Cs_2 molecule are used to obtain relevant difference potential curves in order to describe the origin of diffuse bands and triplet satellite bands. We shall present results from high resolution absorption measurements in cesium cell and emission measurements using pulsed high pressure cesium lamp. Comparison between theoretical predictions and experimental results will be discussed.

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